Note on the Zero-Energy-Limit Solution for the Modified Gross-Pitaevskii Equation

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Abstract

The modified Gross-Pitaevskii equation was derived and solved to obtain the 1D solution in the zero-energy limit. This stationary solution could account for the dominated contributions due to the kinetic effect as well as the chemical potential in inhomogeneous Bose gases.

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Studies of collision phenomena in rather cold gases, e.g., dilute Bose gases, have recently attracted many researchers' attention [1-2]. One relevant research interest is about the solution of the appropriate and modified Gross-Pitaevskii equations for different dimensions [3-4]. New possibilities for observation of macroscopic quantum phenomena arises because of the recent realization of Bose-Einstein condensation in atomic gases [1-2]. There are two important features of the system - weak interaction and significant spatial inhomogeneity. Because of this inhomogeneity a non-trivial *zeroth-order* theory exists, compared to the *first-order* Bogoliubov theory. This theory is based on the mean-field Gross-Pitaevskii equation for the condensate ψ -function. The equation is classical in its essence but contains the $(h/2p)$ constant explicitly. Phenomena such as collective modes, interference, tunneling, Josephson-like current and quantized vortex lines can be described using this equation. The study of deviations from the zeroth-order theory arising from zero-point and thermal fluctuations is also of great interest [5-7]. Thermal fluctuations are described by elementary excitations which define the thermodynamic behaviour of the system and result in Landau-type damping of collective modes.

As a preliminary attempt, followling the mean-field approximate formulation in [3], in this letter, we plan to investigate the 1D solution for the modified Gross-Pitaevski equation in the zero-energy limit. This presentation will give more clues to the studies of the quantum non-equilibrium thermodynamics in inhomogeneous (dilute) Bose gases and the possible appearance of the kinetic mechanism before and/or after Bose-Einstein condensation which is directly linked to the particles (number) density and their energy states or chemical potentials.

The generalization of the Bogoliubov prescription [8] for the ψ-operator to the case of a spatially nonuniform system is

$$\hat{\psi}(\mathbf{r},t) \approx \psi_0(\mathbf{r},t) + \hat{\phi}(\mathbf{r},t) \tag{1}$$

where ψ_0 is the condensate wave function. This is an expression of the second quantization (ψ-operator) for atoms as $n_0 = N_0/V = |\psi_0|^2$ and $\phi \ll \sqrt{n_0}$, N_0 is the number of atoms in

the condensate. To neglect $\hat{\phi}$ means neglecting all correlations and this is a poor approximation when distances between particles are of the order of the effective radius r_e of the atom-atom interaction. To overcome this problem the assumption that the atomic gas is dilute : $n\, r_e^3 \ll 1$ should be made [1-3] ($n = N/V$, N is the number of atoms confined in V). We can use the procedure of the quantum virial expansion to calculate the energy of the system. We have the form

$$E = E_0 + \frac{g}{2}\int n^2(\mathbf{r}) d\mathbf{r}, \tag{2}$$

for the energy of slow particles, where E_0 is the energy of the gas without interaction, $n(\mathbf{r})$ os the density of the gas, $g = 4\pi a\, \hbar^2/m$, a is the s-wave scattering length and m is the particle's mass [3]. After taking into account the correlations (in above equation so that we can neglect $\hat{\phi}$) and considering E as an *effective Hamiltonian* we then have the celebrated Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi_0(\mathbf{r}, t) = [-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + g|\psi_0(\mathbf{r}, t)|^2]\psi_0(\mathbf{r}, t) \tag{3}$$

which describe the dynamics of a non-uniform non-ideal Bose gas at $T = 0$. Here, $V_{ext}(\mathbf{r})$ is the confining potential. If the gas is in its ground state, the time dependence of ψ_0 is given by $\psi_0 \sim \exp(-i\mu t/\hbar)$, where μ is the chemical potential of the gas [1-3]. We thus obtain the form

$$[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + g|\psi_0(\mathbf{r}, t)|^2 - \mu]\psi_0(\mathbf{r}, t) = 0 \tag{4}$$

which could be stationary once t is fixed or selected. We noticed that an equation of above form has been considered before in connection with the theory of superfluidity of liquid helium close to the λ-point [9].

To investigate our interest here, we shall consider the 1D solution of equation (4) for the case of zero-energy limit. Firstly we consider a 3D Bose gas confined tightly in one dimension and weakly in the remaining two dimensions on a length scale l_t ($=\sqrt{\hbar/2m\omega}$ for a harmonic trap of angular frequency of ω). A collision between two condensate particles will typically occur over the characteristic length scale l_{col} once l_t is much larger than l_{col} (thus we can use a local density approximation).

We now model the pair wavefunction of two atoms in the medium by that a single particle with the reduced mass moving in a potential which consists of a circularly symmetric box of radius R and a hard sphere of radius R_a located in the centre of the box. Following the reasoning in the derivation of equation (1), we introduce a similar bias or ghost-effect for $\hat{\phi}$: Ψ which can be relevant to certain critical or kinetic (non-equilibrium) effect (or configurational dissipation) [1-2,5,7,10-11] so that $\mu\,\Psi = \varepsilon$ in the zero-energy, zero-momentum limit. It is presumed that ε still reaches zero in the homogeneous limit. The problem for a 2D $\psi(r, \theta)$ becomes, after referencing to the bias Ψ,

$$[\frac{\partial^2}{\partial r^2} + \frac{\partial}{r\partial r} + \frac{\partial^2}{\partial\theta^2}]\psi = -\varepsilon \tag{5}$$

and, in fact, for a circularly symmetric $\psi(r)$,

$$[\frac{d^2}{dr^2} + \frac{d}{r\, dr}]\psi = -\varepsilon \tag{6}$$

with the boundary conditions : the wave function vanishes on the inner radius ($\psi = 0$ as $r = R_a$), and reaches an asymptotic value at the edge of the box ($\psi \to \Pi$ as $r = R$).
We can obtain the solution

$$\psi(r) = \frac{\varepsilon}{4}[R^2 - r^2 + (R^2 - R_a^2)\frac{\ln(r/R)}{\ln(R/R_a)}] + \Pi\frac{\ln(r/R_a)}{\ln(R/R_a)}, \tag{7}$$

where $R_a \leq r \leq R$. The extra energy caused by the curvature of this wave function resulting from the scattering potential is

$$\Delta E = \frac{\hbar^2}{2m}\int_0^{2\pi}\int_{R_a}^{R}|\nabla\psi(r)|^2 r dr d\theta = \pi\frac{\hbar^2}{m}\{\varepsilon[\frac{R^3 - R_a^3}{12} + \varepsilon\frac{R^2 - R_a^2}{\ln(R/R_a)}(\frac{1}{16} - \frac{R - R_a}{4})] +$$

$$\frac{\Pi}{\ln(R/R_a)}[\Pi + \varepsilon(R - R_a)(\frac{R - R_a}{2} - 1)]\}. \tag{8}$$

Note that, this energy depends upon the size of the box R, which is indeed the length scale relevant for the scattering of two particles in two dimensions [1-3]. The scattering of two particles in a many-body system should obviously not depend on the size of the system as a whole when R becomes large, and so we must interpret R as the physical relevant length scale l_{col}. The appropriate length scale over which a many-body wavefunction changes is the healing length l_h, given in homogeneous Bose condensed systems by $l_h = \hbar/\sqrt{2m\, g_{2D}\, n_0} = \hbar/\sqrt{2m\mu}$ [1-3], and so it is this which must be used in equation (8). We recall that $|\Pi|^2$ corresponds to the condensate density n_0 and the homogeneous limit for a pair interaction strength can still be recovered from above equation.
If we plot $\psi(r)$ w.r.t r (in terms of units of l_t) for different ε (0.0005, 0.001, 0.005, 0.01) and the same Π (0.01) into a figure then the subsequent presentation shows the significant effect of the kinetic part (say, Π) due to ε. The effect of boundary conditions, like Π is minor. From the definition of $\varepsilon = \mu\Psi$, we can understand that the contribution of the chemical potential for ψ of the inhomogeneous gases is indeed dominated, too. We shall investigate more complicated problems [12-13] by the same approach in the future.

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